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Physics of Plasmas

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APPROXIMATE EQUATIONS OF STATE BASED ON PRESSURE EQUILIBRATION  
IN TWO-TEMPERATURE PLASMA MIXTURES

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ABSTRACT

Approximate thermodynamic state relations for multicomponent atomic and molecular gas mixtures are often constructed by artificially partitioning the mixture into its constituent materials, and requiring the separated materials to be in temperature and pressure equilibrium. A numerical algorithm for enforcing this equilibration and computing the resulting approximate state relations in single-temperature mixtures was described in *Phys. Fluids* **21**, 055109 (2009). Here we generalize that algorithm to the case of partially ionized gas mixtures in which the free electrons and heavy particles have different temperatures.

## I. INTRODUCTION

Multicomponent hydrodynamics calculations require thermodynamic state relations for material mixtures. Unfortunately, it is rarely feasible to construct accurate state relations for multicomponent atomic mixtures of interacting materials. In practice, the state relations of the mixture must perforce be approximated in terms of those of the pure materials of which it is comprised. The usual approach [1,2] is to regard the mixture as being artificially partitioned or separated into its constituent components or materials, so that each species or material  $k$  occupies its own compartment or subvolume, which contains some initially undetermined portions of the specific volume and internal energies of the mixture. Different ways of apportioning or distributing the mixture volume and energy among its constituents lead to different approximations. The usual and customary procedure has been to apportion the volume and energy in such a way that the individual materials are in temperature and pressure equilibrium with one another, and to interpret the resulting equilibrated values thereof as the temperature and pressure of the mixture. A practical numerical algorithm for enforcing this equilibration and computing the resulting approximate state relations was described in [2].

The procedure just described provides a tractable and intuitively appealing approximation to the true state relations of the mixture. Unfortunately, that approximation is uncontrolled; i.e., its accuracy cannot readily be quantified or systematically improved. However, its appeal and credibility are considerably enhanced by the fact that it correctly reproduces the exact state relations in mixtures of neutral (non-ionized) ideal gases [1]. This highly desirable property is unfortunately lost in partially ionized gases, but it can easily be restored, at least in principle, by equilibrating the free electron number densities or chemical potentials instead of pressures [1]. In practice, however, this remedy entails significant complications. The free electron number densities or chemical

potentials are not always available, and even when they are their use requires special logic to accommodate both neutral and ionized materials and make a smooth transition between them as the temperature and degree of ionization vary. Moreover, the urgency of implementing this more complicated procedure is reduced by the fact that there are many situations in which pressure equilibration would be expected to produce very similar results. Such situations include those in which the temperature is either sufficiently low that the number density and partial pressure of the free electrons are negligible, or sufficiently high that the free electrons produced by multiple ionization greatly outnumber the heavy particles (ions and neutral atoms). The total pressure of each material is then dominated by the partial pressure of its free electrons, so that equilibrating the former is tantamount to equilibrating the latter, which in turn is equivalent, at least in ideal gases, to equilibrating the free electron number densities or chemical potentials. Conversely, equilibrating pressure, rather than free electron number density or chemical potential, may be less accurate in situations where the number densities of the free electrons and heavy particles are comparable, such as significantly ionized mixtures of the lighter elements.

Thus, although equilibrating free electron number densities or chemical potentials in partially ionized gas mixtures is theoretically preferable to equilibrating pressures [1], it is unfortunately less convenient, the required information is not always available, and in many situations the resulting increased accuracy seems likely to be relatively minor. For these reasons, the common procedure of equilibrating temperatures and pressures remains of practical interest even in partially ionized gases, where it may be employed as a simple expedient in problems where the equilibration of electron number densities or chemical potentials is either infeasible or seems unlikely to produce significantly different results. For this purpose, the algorithm described in [2] can be applied as it stands to single-temperature plasma mixtures, but it requires generalization to deal with two-

temperature plasmas, in which the free electrons and heavy particles have different temperatures. The purpose of this paper is to present that generalization, which is relatively straightforward but somewhat tedious.

Two-temperature plasmas correspondingly possess two internal energies as well, namely the specific internal energies  $E_i$  and  $E_e$  of the heavy particles and electrons, respectively, both of which we define as energies per unit total mass of the mixture, not per unit mass of the heavy particles or electrons. It should be noted that  $E_i$  is not purely thermal but also includes the "cold energy" (i.e., chemical/ionization energy or heat of formation), so in general it does not vanish at zero temperature. In most hydrodynamic calculations the internal energies are determined by energy transport equations, so they constitute independent thermodynamic variables which may be regarded as known quantities for present purposes. In practice, however, one normally solves a transport equation for the total specific internal energy  $E \equiv E_i + E_e$  rather than  $E_i$ , because  $E$  satisfies a simpler equation than  $E_i$  does [3]. One then simply obtains  $E_i$  as  $E_i = E - E_e$ . The other independent thermodynamic variables obtained by solving transport equations, which may therefore also be regarded as known quantities, are the mass density  $\rho$  of the mixture, or equivalently its specific volume  $\xi = 1/\rho$ , and the mass fractions  $Y_k$  of its constituent species or components, which of course must satisfy the constraint  $\sum_k Y_k = 1$ . The artificial partitioning procedure described above then requires that the quantities  $\xi$ ,  $E_i$ , and  $E_e$  be apportioned among the different materials  $k$  in such a way that their pressures and temperatures are equal. In the present context, of course, the heavy particles and electrons have different temperatures which must be separately and independently equilibrated.

The equations that must be solved to implement the procedure described above are of two types: constraint conditions to ensure that the specific volumes and internal energies of the mate-

rials are consistent with the known specific volume and energies of the mixture, and equilibration conditions which ensure pressure and temperature equality among the different materials. These conditions are summarized in Sects. II and III respectively. Together they constitute a closed nonlinear algebraic equation system, which must in general be solved by iterative methods. The Newtonian iteration scheme we use for this purpose is a natural generalization of that described in [2], and is presented, along with a test problem, in Sect. IV. Thermodynamic relations needed to evaluate various partial derivatives for the individual materials and the mixture as a whole in terms of known quantities are given in Sects. V and VI, respectively. The sound speed in the mixture is derived in Sect. VII. The paper is briefly summarized in Sect. VIII.

## II. CONSTRAINT CONDITIONS

For the most part we shall use the same notation as Ref. [2], the main exception being that specific internal energies are denoted by the symbol  $E$  rather than  $e$  so that  $e$  is available for use as a subscript to refer to the electrons. The specific volume of material  $k$  in the artificially partitioned mixture is denoted by  $\xi_k$ , and is defined as the volume occupied by material  $k$  per unit mass of material  $k$ . Thus  $\rho_k \equiv 1/\xi_k$  is the mass density of material  $k$  within its subvolume. The mass of material  $k$  per unit total volume is  $Y_k\rho = Y_k/\xi$  so the volume fraction of material  $k$  in the artificially partitioned mixture is  $v_k = \xi_k Y_k/\xi$ . These volume fractions must of course sum to unity, so that the quantities  $\xi_k$  must satisfy the constraint

$$\sum_{k=1}^N Y_k \xi_k = \xi \quad (1)$$

where  $N$  is the number of materials in the mixture.

The specific internal energies of the heavy particles and electrons of material  $k$  within its subvolume are denoted by  $E_{ik}$  and  $E_{ek}$  respectively, both of which are defined per unit total mass of material  $k$ . The corresponding internal energies of the heavy particles and electrons of material  $k$  per unit mass of the mixture are then simply  $Y_k E_{ik}$  and  $Y_k E_{ek}$ , respectively. These quantities must clearly sum to  $E_i$  and  $E_e$  respectively, so that  $E_{ik}$  and  $E_{ek}$  must satisfy the constraints

$$\sum_{k=1}^N Y_k E_{ik} = E_i \quad (2)$$

$$\sum_{k=1}^N Y_k E_{ek} = E_e \quad (3)$$

### III. EQUILIBRATION CONDITIONS

Equations of state for each pure material  $k$  are required as input to the procedure for determining approximate state relations for the mixture. The basic state relations needed to proceed are the total pressure  $p_k$  and the temperatures  $T_{ik}$  and  $T_{ek}$  of the heavy particles and free electrons, respectively, as functions of the independent thermodynamic variables  $(\xi_k, E_{ik}, E_{ek})$ , and the corresponding inverse relations which express  $\xi_k$ ,  $E_{ik}$ , and  $E_{ek}$  as functions of  $(p_k, T_{ik}, T_{ek})$ . As will be seen below, the present development is based on the latter relations, which must be constructed by combining the state relations for material  $k$  in whatever form they may be available. Many if not most state routines or packages employ temperatures rather than energies as independent thermodynamic variables, in which case  $p_k$ ,  $E_{ik}$ , and  $E_{ek}$  are provided as functions of  $(\xi_k, T_{ik}, T_{ek})$ , or equivalently  $(\rho_k, T_{ik}, T_{ek})$ . Normally  $E_{ik}$  is a function of  $(\xi_k, T_{ik})$  alone and is independent of  $T_{ek}$ , while  $E_{ek}$  is a function of  $(\xi_k, T_{ek})$  alone independently of  $T_{ik}$ . However,  $p_k$  contains contributions from both heavy particles and electrons, and is consequently a function of  $(\xi_k, T_{ik}, T_{ek})$ . The latter contributions are usually assumed to be additive, so that  $p_k = p_{ik} + p_{ek}$ , where  $p_{ik}$  and  $p_{ek}$  are the



heavy-particle and electron pressures, respectively. Normally  $p_{ik}$  is a function of  $(\xi_k, T_{ik})$  alone independently of  $T_{ek}$ , while  $p_{ek}$  is a function of  $(\xi_k, T_{ek})$  alone independently of  $T_{ik}$ . The functional relation  $p_k(\xi_k, T_{ik}, T_{ek})$  can in principle be inverted to obtain  $\xi_k$  as a function of  $(p_k, T_{ik}, T_{ek})$ , and the resulting expression can then be substituted into  $E_{ik}(\xi_k, T_{ik})$  and  $E_{ek}(\xi_k, T_{ek})$  to obtain the functions  $E_{ik}(p_k, T_{ik}, T_{ek})$  and  $E_{ek}(p_k, T_{ik}, T_{ek})$ . Similarly, the functional relations  $p_{ik}(\xi_k, T_{ik})$  and  $p_{ek}(\xi_k, T_{ek})$  can in principle be inverted to obtain  $\xi_k$  as a function of either  $(p_{ik}, T_{ik})$  or  $(p_{ek}, T_{ek})$ , and those expressions can be substituted into  $E_{ik}(\xi_k, T_{ik})$  and  $E_{ek}(\xi_k, T_{ek})$  to obtain the functions  $E_{ik}(p_{ik}, T_{ik})$  and  $E_{ek}(p_{ek}, T_{ek})$ .

In accordance with the discussion of Sect. I, the equilibration conditions that we impose to implicitly determine the quantities  $\xi_k$ ,  $E_{ik}$ , and  $E_{ek}$  are as follows:

$$p_k(\xi_k, T_i, T_e) = p \quad (4)$$

$$T_{ik}(\xi_k, E_{ik}) = T_i \quad (5)$$

$$T_{ek}(\xi_k, E_{ek}) = T_e \quad (6)$$

Equations (1)–(6) constitute a system of  $3N + 3$  equations in the  $3N + 3$  unknown quantities  $\xi_k$ ,  $E_{ik}$ ,  $E_{ek}$ ,  $p$ ,  $T_i$ , and  $T_e$ . This system is highly nonlinear and must in general be solved by iterative methods. A suitable iteration scheme for this purpose is described in the next section.

#### IV. NEWTONIAN ITERATION SCHEME

Let  $\eta$  be the iteration index, which will be displayed as a superscript. Thus the approximate value of any quantity  $q$  after iteration  $\eta$  but before iteration  $\eta + 1$  is denoted by  $q^\eta$ . The iteration scheme defines how the quantities  $\xi_k$ ,  $E_{ik}$ ,  $E_{ek}$ ,  $p$ ,  $T_i$ , and  $T_e$  are advanced from iteration  $\eta$  to

iteration  $\eta + 1$ . This will be done by means of linearized approximations to Eqs. (1)–(6). The constraint Eqs. (1)–(3) are already linear, so they become

$$\sum_{k=1}^N Y_k \xi_k^{\eta+1} = \xi \quad (7)$$

$$\sum_{k=1}^N Y_k E_{ik}^{\eta+1} = E_i \quad (8)$$

$$\sum_{k=1}^N Y_k E_{ek}^{\eta+1} = E_e \quad (9)$$

The remainder of the scheme is defined by writing linearized approximations for the changes in  $\xi_k$ ,  $E_{ik}$ , and  $E_{ek}$  from iteration  $\eta$  to iteration  $\eta + 1$  required to produce values of  $p_k^{\eta+1}$ ,  $T_{ik}^{\eta+1}$ , and  $T_{ek}^{\eta+1}$  that satisfy Eqs. (4)–(6):

$$\xi_k^{\eta+1} - \xi_k^\eta = \left( \frac{\partial \xi_k}{\partial p_k} \right) (p_k^{\eta+1} - p_k^\eta) + \left( \frac{\partial \xi_k}{\partial T_{ik}} \right) (T_i^{\eta+1} - T_{ik}^\eta) + \left( \frac{\partial \xi_k}{\partial T_{ek}} \right) (T_e^{\eta+1} - T_{ek}^\eta) \quad (10)$$

$$E_{ik}^{\eta+1} - E_{ik}^\eta = \left( \frac{\partial E_{ik}}{\partial p_k} \right) (p_k^{\eta+1} - p_k^\eta) + \left( \frac{\partial E_{ik}}{\partial T_{ik}} \right) (T_i^{\eta+1} - T_{ik}^\eta) + \left( \frac{\partial E_{ik}}{\partial T_{ek}} \right) (T_e^{\eta+1} - T_{ek}^\eta) \quad (11)$$

$$E_{ek}^{\eta+1} - E_{ek}^\eta = \left( \frac{\partial E_{ek}}{\partial p_k} \right) (p_k^{\eta+1} - p_k^\eta) + \left( \frac{\partial E_{ek}}{\partial T_{ik}} \right) (T_i^{\eta+1} - T_{ik}^\eta) + \left( \frac{\partial E_{ek}}{\partial T_{ek}} \right) (T_e^{\eta+1} - T_{ek}^\eta) \quad (12)$$

where it is understood that partial derivatives with respect to any of the variables  $(p_k, T_{ik}, T_{ek})$  are taken with the other two held constant, and are evaluated at iteration  $\eta$ . Since all quantities are presumed known at the previous iteration  $\eta$ , Eqs. (7)–(12) constitute a determinate system of  $3N + 3$  equations in the  $3N + 3$  unknown quantities  $\xi_k^{\eta+1}$ ,  $E_{ik}^{\eta+1}$ ,  $E_{ek}^{\eta+1}$ ,  $p_k^{\eta+1}$ ,  $T_i^{\eta+1}$ , and  $T_e^{\eta+1}$ . It is apparent by inspection that if the iteration converges as  $\eta \rightarrow \infty$ , it produces a solution of Eqs. (1)–(6).

Substituting Eqs. (10)–(12) into Eqs. (7)–(9), we obtain

$$A_{pp}p^{\eta+1} + A_{pi}T_i^{\eta+1} + A_{pe}T_e^{\eta+1} = B_p \quad (13)$$

$$A_{ip}p^{\eta+1} + A_{ii}T_i^{\eta+1} + A_{ie}T_e^{\eta+1} = B_i \quad (14)$$

$$A_{ep}p^{\eta+1} + A_{ei}T_i^{\eta+1} + A_{ee}T_e^{\eta+1} = B_e \quad (15)$$

where

$$A_{pp} = \sum_k Y_k \left( \frac{\partial \xi_k}{\partial p_k} \right) ; \quad A_{pi} = \sum_k Y_k \left( \frac{\partial \xi_k}{\partial T_{ik}} \right) ; \quad A_{pe} = \sum_k Y_k \left( \frac{\partial \xi_k}{\partial T_{ek}} \right) \quad (16)$$

$$A_{ip} = \sum_k Y_k \left( \frac{\partial E_{ik}}{\partial p_k} \right) ; \quad A_{ii} = \sum_k Y_k \left( \frac{\partial E_{ik}}{\partial T_{ik}} \right) ; \quad A_{ie} = \sum_k Y_k \left( \frac{\partial E_{ik}}{\partial T_{ek}} \right) \quad (17)$$

$$A_{ep} = \sum_k Y_k \left( \frac{\partial E_{ek}}{\partial p_k} \right) ; \quad A_{ei} = \sum_k Y_k \left( \frac{\partial E_{ek}}{\partial T_{ik}} \right) ; \quad A_{ee} = \sum_k Y_k \left( \frac{\partial E_{ek}}{\partial T_{ek}} \right) \quad (18)$$

$$B_p = \xi - \sum_k Y_k \xi_k^\eta + \sum_k Y_k \left[ p_k^\eta \left( \frac{\partial \xi_k}{\partial p_k} \right) + T_{ik}^\eta \left( \frac{\partial \xi_k}{\partial T_{ik}} \right) + T_{ek}^\eta \left( \frac{\partial \xi_k}{\partial T_{ek}} \right) \right] \quad (19)$$

$$B_i = E_i - \sum_k Y_k E_{ik}^\eta + \sum_k Y_k \left[ p_k^\eta \left( \frac{\partial E_{ik}}{\partial p_k} \right) + T_{ik}^\eta \left( \frac{\partial E_{ik}}{\partial T_{ik}} \right) + T_{ek}^\eta \left( \frac{\partial E_{ik}}{\partial T_{ek}} \right) \right] \quad (20)$$

$$B_e = E_e - \sum_k Y_k E_{ek}^\eta + \sum_k Y_k \left[ p_k^\eta \left( \frac{\partial E_{ek}}{\partial p_k} \right) + T_{ik}^\eta \left( \frac{\partial E_{ek}}{\partial T_{ik}} \right) + T_{ek}^\eta \left( \frac{\partial E_{ek}}{\partial T_{ek}} \right) \right] \quad (21)$$

The thermodynamic derivatives in Eqs. (16)–(21) must be evaluated in terms of the particular state relations and routines available to the user. As mentioned in Sect. III, most such routines employ the independent thermodynamic variables  $(\rho_k, T_{ik}, T_{ek})$  rather than  $(p_k, T_{ik}, T_{ek})$ . The thermodynamic identities needed to evaluate the partial derivatives in Eqs. (16)–(21) in terms of derivatives with respect to  $(\rho_k, T_{ik}, T_{ek})$  are summarized in Sect. V.

Equations (13)–(15) are a system of three linear equations in the three unknown quantities  $p^{\eta+1}$ ,  $T_i^{\eta+1}$ , and  $T_e^{\eta+1}$ , the solution to which is readily obtained from Cramer's rule. To minimize

multiplications, it is convenient to compute the minors of the matrix  $A$  at the outset and save them for repeated use. These quantities are given by

$$M_{pp} = A_{ii}A_{ee} - A_{ei}A_{ie} \quad (22)$$

$$M_{ip} = A_{pi}A_{ee} - A_{ei}A_{pe} \quad (23)$$

$$M_{ep} = A_{pi}A_{ie} - A_{ii}A_{pe} \quad (24)$$

$$M_{pi} = A_{ip}A_{ee} - A_{ep}A_{ie} \quad (25)$$

$$M_{ii} = A_{pp}A_{ee} - A_{ep}A_{pe} \quad (26)$$

$$M_{ei} = A_{pp}A_{ie} - A_{ip}A_{pe} \quad (27)$$

$$M_{pe} = A_{ip}A_{ei} - A_{ep}A_{ii} \quad (28)$$

$$M_{ie} = A_{pp}A_{ei} - A_{ep}A_{pi} \quad (29)$$

$$M_{ee} = A_{pp}A_{ii} - A_{ip}A_{pi} \quad (30)$$

According to Cramer's rule, the solution of Eqs. (13)–(15) is then given by

$$p^{\eta+1} = R D_p \quad (31)$$

$$T_i^{\eta+1} = R D_i \quad (32)$$

$$T_e^{\eta+1} = R D_e \quad (33)$$

where

$$D_p = B_p M_{pp} - B_i M_{ip} + B_e M_{ep} \quad (34)$$

$$D_i = -B_p M_{pi} + B_i M_{ii} - B_e M_{ei} \quad (35)$$

$$D_e = B_p M_{pe} - B_i M_{ie} + B_e M_{ee} \quad (36)$$

$$R = 1/(A_{pp} M_{pp} - A_{pi} M_{pi} + A_{pe} M_{pe}) \quad (37)$$

Equations (31)–(33) combine with Eqs. (10)–(12) to provide explicit expressions for  $\xi_k^{\eta+1}$ ,  $E_{ik}^{\eta+1}$ , and  $E_{ek}^{\eta+1}$ , which in turn determine  $p_k^{\eta+1}$ ,  $T_{ik}^{\eta+1}$ , and  $T_{ek}^{\eta+1}$  via the individual material state relations.

Newtonian iteration schemes are notoriously vulnerable to overshoots, so limiters are sometimes necessary to ensure convergence. Experience in applying the above iteration scheme on a variety of problems has shown that divergence is usually avoided if  $\xi_k^{\eta+1}$  is not allowed to differ from  $\xi_k^\eta$  by more than a factor of two. Limiters could also be applied to  $E_{ik}^{\eta+1}$  and  $E_{ek}^{\eta+1}$ , but this has not been found necessary except when the initial guesses are very far off.

The iteration procedure is normally initialized by setting  $\xi_k^0$ ,  $E_{ik}^0$ , and  $E_{ek}^0$  equal to their values from the previous time step. Note that there is no need to initialize  $p$ ,  $T_i$ , or  $T_e$  since Eqs. (10)–(12) do not involve  $p^\eta$ ,  $T_i^\eta$ , or  $T_e^\eta$ . The iteration is continued until  $\max(\epsilon_{pk}^\eta, \epsilon_{ik}^\eta, \epsilon_{ek}^\eta) < \epsilon$  for all  $k$ , where  $\epsilon \approx 10^{-4}$  and

$$\epsilon_{pk}^\eta \equiv |Y_k(1 - p_k^\eta/p^\eta)| \quad (38)$$

$$\epsilon_{ik}^\eta \equiv |Y_k(1 - T_{ik}^\eta/T_i^\eta)| \quad (39)$$

$$\epsilon_{ek}^\eta \equiv |Y_k(1 - T_{ek}^\eta/T_e^\eta)| \quad (40)$$

To illustrate the behavior of the iteration algorithm, we applied the above procedure to a mixture of materials commonly used in inertial confinement fusion capsules, namely Hydrogen (H), Carbon (C), Oxygen (O), Silicon (Si) and Germanium (Ge). The mixture consists of 20% by

mass fraction of each element ( $Y_k = 0.2$  for  $k = 1, \dots, 5$ ). The density, total energy and electron energy are  $\rho = 100$  (g/cc),  $E = 10^{15}$  (erg/g) and  $E_e = 10^{12}$  (erg/g), respectively. These conditions correspond to a wide separation in ion and electron temperatures, which tests the robustness of the equilibration algorithm. Starting guesses for species densities and energies are  $\rho_k = \rho$ ,  $E_{ik} = E - E_e$  and  $E_{ek} = E_e$ . The convergence of the solution method is shown in Fig. 1. It takes only three iterations to bring the mixture into pressure and temperature equilibrium, despite the large (factor of six) changes in species quantities.

Other tests show that the method works well at high temperatures, where thermodynamic derivatives are smooth, but can run into trouble at low temperatures where  $(\partial p_k / \partial \rho_k)$  can pass through zero (e.g., phase changes), and  $E_e$  and its derivatives go to zero and/or become unreliable due to deficiencies in the electronic state relations when ionization is negligible (e.g., neutral gases). A workaround for these situations is to put floors  $p_0$  and  $E_{e0}$  under  $p_k$  and  $E_{ek}$ , such that  $\partial p_k / \partial \rho_k \geq p_0 / \rho_k$  and  $\partial E_{ek} / \partial T_{ek} \geq E_{e0} / T_{ek}$ . This reduces the accuracy of the method at low temperatures, but has been found sufficient for problems with strong heating in which energies quickly increase by several orders of magnitude.

## V. THERMODYNAMIC DERIVATIVES OF THE INDIVIDUAL MATERIALS

The following thermodynamic identities can be derived by the usual straightforward but tedious manipulations. In this section, but only herein, all subscripts  $k$  will be suppressed for simplicity, with the understanding that the relations below apply separately to each material  $k$  in the mixture, and the subscripts  $k$  must of course be restored before these relations may be used in Eqs. (16)–(21). (The relations below also apply as they stand to the mixture as a whole, but are not useful in that context because the corresponding derivatives for the mixture are simply given by

Eqs. (53)–(55) in Sect. VI below.) In what follows, a subscript  $T$  indicates that both  $T_i$  and  $T_e$  are held constant, and it is understood that partial derivatives with respect to either  $T_i$  or  $T_e$  are always taken with the other held constant, even though this is not explicitly indicated by a subscript.

$$\left(\frac{\partial \xi}{\partial p}\right)_T = -\frac{1}{\rho^2} \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (41)$$

$$\left(\frac{\partial E_i}{\partial p}\right)_T = \left(\frac{\partial E_i}{\partial \rho}\right)_T \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (42)$$

$$\left(\frac{\partial E_e}{\partial p}\right)_T = \left(\frac{\partial E_e}{\partial \rho}\right)_T \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (43)$$

$$\left(\frac{\partial \xi}{\partial T_i}\right)_p = \frac{1}{\rho^2} \left(\frac{\partial p}{\partial T_i}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (44)$$

$$\left(\frac{\partial E_i}{\partial T_i}\right)_p = \left(\frac{\partial E_i}{\partial T_i}\right)_\rho - \left(\frac{\partial E_i}{\partial \rho}\right)_T \left(\frac{\partial p}{\partial T_i}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (45)$$

$$\left(\frac{\partial E_e}{\partial T_i}\right)_p = \left(\frac{\partial E_e}{\partial T_i}\right)_\rho - \left(\frac{\partial E_e}{\partial \rho}\right)_T \left(\frac{\partial p}{\partial T_i}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (46)$$

$$\left(\frac{\partial \xi}{\partial T_e}\right)_p = \frac{1}{\rho^2} \left(\frac{\partial p}{\partial T_e}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (47)$$

$$\left(\frac{\partial E_i}{\partial T_e}\right)_p = \left(\frac{\partial E_i}{\partial T_e}\right)_\rho - \left(\frac{\partial E_i}{\partial \rho}\right)_T \left(\frac{\partial p}{\partial T_e}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (48)$$

$$\left(\frac{\partial E_e}{\partial T_e}\right)_p = \left(\frac{\partial E_e}{\partial T_e}\right)_\rho - \left(\frac{\partial E_e}{\partial \rho}\right)_T \left(\frac{\partial p}{\partial T_e}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_T^{-1} \quad (49)$$

If  $E_e$  is independent of  $T_i$  and  $E_i$  is independent of  $T_e$  at constant  $\rho$ , which is normally the case for the individual materials  $k$ , then the first term in the right members of Eqs. (46) and (48) vanishes and may be omitted. Even when these conditions are satisfied, however, the corresponding terms do not in general vanish for the mixture as a whole.

## VI. THERMODYNAMIC DERIVATIVES OF THE MIXTURE

The iteration scheme determines the mixture state relations for the dependent thermody-

namic variables  $(p, T_i, T_e)$  as functions of the independent thermodynamic variables  $(\rho, E_i, E_e)$ . To obtain the mixture specific heats, and for various other purposes, it is necessary to evaluate partial derivatives of the mixture state relations. In this section we derive the thermodynamic relations needed to evaluate the partial derivatives of  $(\rho, E_i, E_e)$  with respect to  $(p, T_i, T_e)$ , as well as the derivatives of  $(p, E_i, E_e)$  with respect to  $(\rho, T_i, T_e)$ .

Partial derivatives of the state relations for the mixture may be obtained by taking the differentials of the constraint conditions of Eqs. (1)–(3) and the equilibration conditions of Eqs. (4)–(6) with respect to  $(p, T_i, T_e)$  and combining the results. We thereby obtain

$$d\xi = A_{pp}dp + A_{pi}dT_i + A_{pe}dT_e \quad (50)$$

$$dE_i = A_{ip}dp + A_{ii}dT_i + A_{ie}dT_e \quad (51)$$

$$dE_e = A_{ep}dp + A_{ei}dT_i + A_{ee}dT_e \quad (52)$$

where the quantities  $A_{\alpha\beta}$  are the final converged values of the matrix elements defined in Eqs. (16)–(18). It follows that

$$\left(\frac{\partial \xi}{\partial p}\right)_T = A_{pp}; \quad \left(\frac{\partial \xi}{\partial T_i}\right)_p = A_{pi}; \quad \left(\frac{\partial \xi}{\partial T_e}\right)_p = A_{pe} \quad (53)$$

$$\left(\frac{\partial E_i}{\partial p}\right)_T = A_{ip}; \quad \left(\frac{\partial E_i}{\partial T_i}\right)_p = A_{ii}; \quad \left(\frac{\partial E_i}{\partial T_e}\right)_p = A_{ie} \quad (54)$$

$$\left(\frac{\partial E_e}{\partial p}\right)_T = A_{ep}; \quad \left(\frac{\partial E_e}{\partial T_i}\right)_p = A_{ei}; \quad \left(\frac{\partial E_e}{\partial T_e}\right)_p = A_{ee} \quad (55)$$

These relations may be transformed into expressions for the derivatives of  $(p, E_i, E_e)$  with respect



to  $(\rho, T_i, T_e)$  by means of further straightforward but tedious manipulations. The net results are

$$\left(\frac{\partial p}{\partial \rho}\right)_T = -\frac{1}{\rho^2 A_{pp}}; \quad \left(\frac{\partial p}{\partial T_i}\right)_\rho = -\frac{A_{pi}}{A_{pp}}; \quad \left(\frac{\partial p}{\partial T_e}\right)_\rho = -\frac{A_{pe}}{A_{pp}} \quad (56)$$

$$\left(\frac{\partial E_i}{\partial \rho}\right)_T = -\frac{A_{ip}}{\rho^2 A_{pp}}; \quad \left(\frac{\partial E_i}{\partial T_i}\right)_\rho = A_{ii} - \frac{A_{ip}A_{pi}}{A_{pp}}; \quad \left(\frac{\partial E_i}{\partial T_e}\right)_\rho = A_{ie} - \frac{A_{ip}A_{pe}}{A_{pp}} \quad (57)$$

$$\left(\frac{\partial E_e}{\partial \rho}\right)_T = -\frac{A_{ep}}{\rho^2 A_{pp}}; \quad \left(\frac{\partial E_e}{\partial T_i}\right)_\rho = A_{ei} - \frac{A_{ep}A_{pi}}{A_{pp}}; \quad \left(\frac{\partial E_e}{\partial T_e}\right)_\rho = A_{ee} - \frac{A_{ep}A_{pe}}{A_{pp}} \quad (58)$$

## VII. THE SOUND SPEED

In this section we derive the sound speed of the mixture in the limit of slow energy exchange between heavy particles and electrons. The usual thermodynamic expressions for sound speed are not directly applicable in two-temperature plasmas, where there are three rather than two independent thermodynamic variables. In this situation, the simplest way to proceed is to go back to basics and directly determine the sound speed by linearizing the two-temperature hydrodynamic equations about a uniform steady state. We shall restrict attention to the case in which the rate of energy exchange between heavy particles and electrons is negligible. Under these conditions, the relation between acoustic variations in pressure and density can be inferred from the adiabatic thermodynamic relations

$$dp = K_\rho d\rho + K_i dE_i + K_e dE_e \quad (59)$$

$$dE_i = \frac{p_i}{\rho^2} d\rho \quad (60)$$

$$dE_e = \frac{p_e}{\rho^2} d\rho \quad (61)$$

where  $p_e = \sum_k v_k p_{ek}$  is the partial pressure of the free electrons,  $p_i = p - p_e$ , and

$$K_\rho = \left( \frac{\partial p}{\partial \rho} \right)_{E_i, E_e} \quad (62)$$

$$K_i = \left( \frac{\partial p}{\partial E_i} \right)_{\rho, E_e} \quad (63)$$

$$K_e = \left( \frac{\partial p}{\partial E_e} \right)_{\rho, E_i} \quad (64)$$

The electron pressures  $p_{ek}$  are determined as functions of  $(\xi_k, T_e)$  by the thermodynamic state relations of the individual materials  $k$ . In contrast to the total pressures  $p_k$ , the electron pressures  $p_{ek}$  are not equilibrated, so they will in general be unequal and must be volume-weighted as indicated above to obtain  $p_e$  for the mixture [1]. Combining Eqs. (59)–(61), we obtain

$$dp = c^2 d\rho \quad (65)$$

where

$$\rho^2 c^2 = \rho^2 K_\rho + p_i K_i + p_e K_e \quad (66)$$

The linearized hydrodynamic equations in one spatial dimension  $x$  reduce to

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial u}{\partial x} \quad (67)$$

$$\rho \frac{\partial u}{\partial t} = -\frac{\partial p}{\partial x} \quad (68)$$

where  $u$  is the fluid velocity. Combining Eqs. (65), (67), and (68), we obtain

$$\frac{\partial^2 \rho}{\partial t^2} = c^2 \frac{\partial^2 \rho}{\partial x^2} \quad (69)$$

which is just the familiar wave equation in one dimension, thereby confirming that  $c$  as determined by Eq. (66) is indeed the sound speed.

The derivatives  $K_\rho$ ,  $K_i$ , and  $K_e$  are simply related to quantities that have already been evaluated during the iteration. Equations (50)–(52) are a linear system of the same form as Eqs. (13)–(15), with  $(B_p, B_i, B_e)$  replaced by  $(d\xi, dE_i, dE_e)$  and  $(p, T_i, T_e)^{\eta+1}$  replaced by  $(dp, dT_i, dT_e)$ . It then follows from Eqs. (31) and (34) that

$$dp = R(M_{pp}d\xi - M_{ip}dE_i + M_{ep}dE_e) \quad (70)$$

Comparison with Eq. (59) shows that

$$\rho^2 K_\rho = -RM_{pp} \quad (71)$$

$$K_i = -RM_{ip} \quad (72)$$

$$K_e = RM_{ep} \quad (73)$$

which combine with Eq. (66) to yield

$$\rho^2 c^2 = R(-M_{pp} - p_i M_{ip} + p_e M_{ep}) \quad (74)$$

## VIII. SUMMARY

We have presented an iterative algorithm for determining pressure, ion temperature and electron temperature given the density, total energy and electron energy of a plasma mixture. By solving a  $3N + 3$  system of equations, all species are brought into pressure and temperature equi-

librium, with ions equilibrated separately from electrons. The algorithm has been applied to a variety of inertial confinement fusion problems and found to converge rapidly, provided the electron temperature is sufficiently high for significant ionization. The sound speed and specific heats of the plasma mixture are easily computed after the equilibration procedure.

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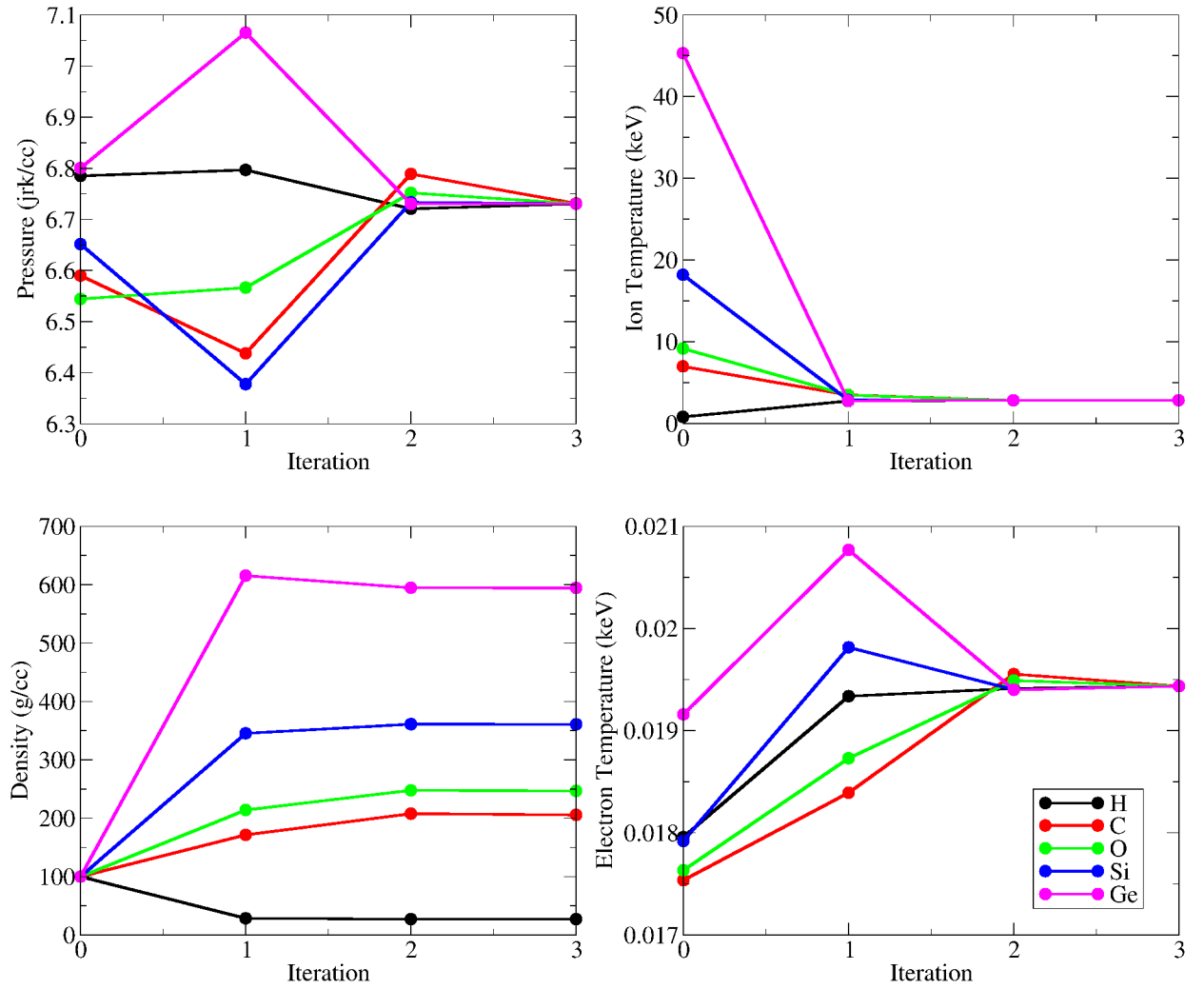


Figure 1: Convergence of species densities, total pressures, ion temperatures and electron temperatures during the course of Newton-Raphson iteration.